

# Molprobit Assignment

Your Mentor:

Mike Easton



Pseudoknot

- Use Molprobit to analyze 28 possible pseudoknot structures
- Fill out the vdsclass google spreadsheet of your 28 assigned structures
- Upload the results file to VDS Biooproject folder on gdocs

What you will  
be doing

# Step 1: Wikispaces

Wiki Home  
 Projects  
 Pages and Files  
 Members  
 Recent Changes  
 Manage Wiki  
 Search Wiki

Home  
 Announcements Page  
 Google Calendar  
 Class Picture  
 Mini Research Write Ups  
 PseudoKnot Project  
 Research Pages (old)  
 Targets  
 The Random Walk  
 Syllabus VDS Spring12  
 – see BB for complete Syllabus  
 Mentors  
 Calendar for Staff

## ★ PseudoKnot Project

Edit 2 0

### RNA Pseudoknot Project

#### Aims:

- find binders to an RNA pseudoknot for anti-viral potential
  - validation dock of biotin to an aptamer pseudoknot - in PDB already (<http://www.rcsb.org/pdb/explore/explore.do?structureId=1F27>)
  - set up RNA receptor, assess model on MolProbability
  - prepare ligands - generate tautomers, convert to 3D, minimize (in ICM or Babel)

#### Instructions for Using Molprobability to Analyze Structure:

- Find Structures here: [https://docs.google.com/open?id=0B\\_Gl3lMyhDsoYTEyNzJhMWEtMDA2Ny00Y2U3LTgzM2ltZWE1MTImNmM4MmUz](https://docs.google.com/open?id=0B_Gl3lMyhDsoYTEyNzJhMWEtMDA2Ny00Y2U3LTgzM2ltZWE1MTImNmM4MmUz)
- Find assigned structures and download
- Go to : <http://molprobability.biochem.duke.edu/>
- On the **Browse** button - go find your .pdb file.
- Hit '**Upload**'
- You will see a short page of some results and hopefully see an image on the right hand side (rhs), hit '**Continue**'
- Analyze all-atom contacts and geometry
- Use defaults that are already selected --> '**Run programs to perform these analyses**'
- Input Data in to the Gdocs spreadsheet under the folder Vdsbiooproject
- Go back to the Molprobability and Click '**Multi-criterion chart**'
- To save a copy of the page, in your web browser go to File >> Save As >> Web Page complete
- give it a name that corresponds to the structure you have analyzed. For example: **structure-0016.htm**
- Save this file to your desktop and then upload it to the Gdocs folder VDSbiooproject at the bottom as shown
- You will need to open a new Molprobability for each structure

Go to wikispaces and click on Pseudoknot Project

Click the Gdocs link and find your Structures. Download them

Click the link to go to the Molprobability Website:

<http://molprobability.biochem.duke.edu/>

# Step 2: Molprobability



## Main page

Evaluate X-ray  
Evaluate NMR  
Fix up structure  
Work with kins

View & download files  
Lab notebook  
Feedback & bugs  
Site map

Save session  
Log out

You are using 0% of  
your 200 Mb of disk  
space.

## FILE UPLOAD/RETRIEVAL ([MORE OPTIONS](#))

PDB/NDB code:

type:

No file chosen

type:

## Walk-thrus & tutorials:

**Evaluate X-ray structure:** Typical steps for a published X-ray crystal structure or one still undergoing refinement.

**Evaluate NMR structure:** Typical steps for a published NMR ensemble or one still undergoing refinement.

**Fix up structure:** Rebuild the model to remove outliers as part of the refinement cycle.

**Work with kinemages:** Create and view interactive 3-D graphics from your web browser.

## What's new in 3.19:

- [JifliLoop](#) moved to main page, more options enabled.

## Common questions:

**Cite MolProbity:** Chen et al. (2010) MolProbity: all-atom structure validation for macromolecular crystallography. Acta Crystallographica D66:12-21.

and/or

Davis et al. (2007) MolProbity: all-atom contacts and structure validation for proteins and nucleic acids. Nucleic Acids Research 35:W375-W383.

**Cite KiNG:** Chen et al. (2009) KiNG (Kinemage, Next Generation): A versatile interactive molecular and scientific visualization program. Protein Science 18:2403-2407.

**Installing Java:** how to make kinemage graphics work in your browser.

**Download MolProbity:** how can I run a private MolProbity server, or run from the command line?

*NB: the back button doesn't work inside MolProbity*

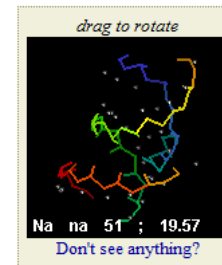
About [MolProbity](#) | Website for [the Richardson Lab](#) | Internal reference 3.19

Click upload

Choose the structure to  
analyze

Your file from local disk was uploaded as structure-0001.pdb.

- 1 chain(s) is/are present [1 unique chain(s)]
- A total of 30 residues are present.
- 30 nucleic acid residues are present.
- Explicit hydrogens are present.
- 30 hetero group(s) is/are present.
- 0 PDBv2.3 atoms were found. Proceeding assuming PDBv3 formatted file.



Continue >

About [MolProbity](#) | Website for [the Richardson Lab](#) | Internal reference 3.19

Click continue

Wait for the file to upload and  
this page will appear



## Main page

Evaluate X-ray  
Evaluate NMR  
Fix up structure  
Work with kins

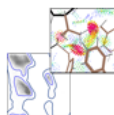
View & download files  
Lab notebook  
Feedback & bugs  
Site map

Save session  
Log out

You are using 0% of  
your 200 Mb of disk  
space.

### SUGGESTED TOOLS (ALL TOOLS)

Currently working on: **structure-0001.pdb**



Analyze all-atom contacts and geometry



Visualize interface contacts



Add hydrogens



Make simple kinemages



Edit PDB file



Downgrade file to PDBv2.3 format (for download only)



Fill gaps in protein backbone with JiffiLoop (beta test)

### RECENTLY GENERATED RESULTS (ALL RESULTS)



Uploaded PDB file as structure-0001.pdb

12:35am EST

[set time zone]

### POPULAR DOWNLOADS (ALL DOWNLOADS)

	File name	Size	View...	Download
<input type="checkbox"/>	> coordinates			
<input type="checkbox"/>	> kinemages			

Another loading page  
appears, wait and this  
page will show up

Click on Analyze all-atom contacts  
and geometry

## Summary statistics

All-Atom Contacts	Clashscore, all atoms:	15.18	49 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.		
Nucleic Acid Geometry	Probably wrong sugar puckers:	1	Goal: 0
	Bad backbone conformations#:	9	Goal: 0
	Residues with bad bonds:	10.00%	Goal: 0%
	Residues with bad angles:	86.67%	Goal: <0.1%

\* 100<sup>th</sup> percentile is the best among structures of comparable resolution; 0<sup>th</sup> percentile is the worst.

# RNA backbone was recently shown to be rotameric. Outliers are RNA suites that don't fall into recognized rotamers.

## Multi-criterion visualizations



Multi-criterion  
kinemage

[View in KiNG](#) | [Download](#) (260 Kb)



Multi-criterion  
chart

[View](#) (45 Kb)

Input this data into the google  
docs spreadsheet:

### All-Atom Contacts

- Clashscore, all atoms
- percentile

### Nucleic Acid Geometry

- Probably wrong sugar puckers
- Bad backbone conformations#
- Residues with bad bonds
- Residues with bad angles

**DO NOT CLOSE**  
**THIS**  
**WINDOW!**

# Step 3: Google Docs

Google

VDS Biooproject x

Docs

CREATE

Home

Starred


Owned by me

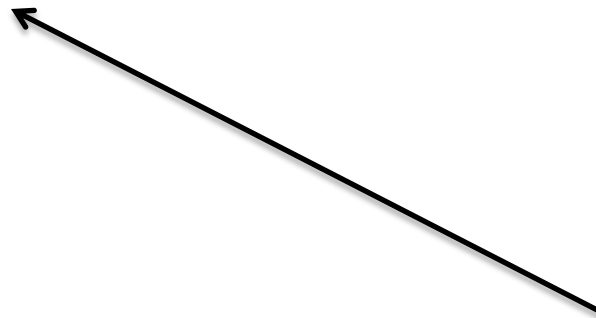
All items

Trash

My collections

- ADAM NGUYEN
- CH379H
- GroupMeetingSlides
- JournalClub
- Mentors
- Misc
- Pics
- Protocols
- Results&Data
- StudentFolders
- VDS Biooproject**  
No collections

<input type="checkbox"/>	TITLE
<input type="checkbox"/> ☆	 VDS Pseudoknot Shared



Click on this spreadsheet, find your structures and input the data

Login into the vdsclass gdocs and click on this folder



## Summary statistics

All-Atom Contacts	Clashscore, all atoms:	15.18	49 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.		
Nucleic Acid Geometry	Probably wrong sugar puckers:	1	Goal: 0
	Bad backbone conformations <sup>#</sup> :	9	Goal: 0
	Residues with bad bonds:	10.00%	Goal: 0%
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\* 100<sup>th</sup> percentile is the best among structures of comparable resolution; 0<sup>th</sup> percentile is the worst.

<sup>#</sup> RNA backbone was recently shown to be rotameric. Outliers are RNA suites that don't fall into recognized rotamers.

## Multi-criterion visualizations



Multi-criterion  
kinemage

[View in KiNG](#) | [Download \(260 Kb\)](#)



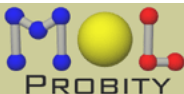
Multi-criterion  
chart

[View \(45 Kb\)](#)

Go back to your  
molprobity page



Click on the Multi-criterion chart link



## Viewing structure-0001-multi.table

When finished, you should [close this window](#).

Hint: Use File | Save As... to save a copy of this page.

All-Atom Contacts	Clashscore, all atoms:	15.18	49 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.		
Nucleic Acid Geometry	Probably wrong sugar puckers:	1	Goal: 0
	Bad backbone conformations <sup>#</sup> :	9	Goal: 0
	Residues with bad bonds:	10.00%	Goal: 0%
	Residues with bad angles:	86.67%	Goal: <0.1%

\* 100<sup>th</sup> percentile is the best among structures of comparable resolution; 0<sup>th</sup> percentile is the worst.

<sup>#</sup> RNA backbone was recently shown to be rotameric. Outliers are RNA suites that don't fall into recognized rotamers.

#	Res	High B	Clash > 0.4Å	Base-P perp. dist.	RNA suite conf.	Bond lengths.	Bond angles.
		Avg: 0.00	Clashscore: 15.18	Outliers: 1 of 30	Outliers: 9 of 30	Outliers: 3 of 30	Outliers: 26 of 30
A 1	U	0	-	-	conformer: __ &delta;&delta;&gamma none (incomplete)	-	2 OUTLIER(S) worst is C3'-C2'-C1': -5.669 &sigma
A 2	C	0	-	-	conformer: 1a &delta;&delta;&gamma 33 p, suiteness = 0.516	-	2 OUTLIER(S) worst is O4'-C1'-N19: 6.209 &sigma
A 3	A	0	-	-	conformer: 1a &delta;&delta;&gamma 33 p, suiteness = 0.651	-	2 OUTLIER(S) worst is O4'-C1'-N19: 5.498 &sigma
A 4	G	0	-	-	conformer: 1c &delta;&delta;&gamma 33 t, suiteness = 0.54	-	1 OUTLIER(S) worst is OP1-P-OP2: -4.347 &sigma
A 5	G	0	0.452Å H2' with A 6 C C6	-	conformer: 1a &delta;&delta;&gamma 33 p, suiteness = 0.604	1 OUTLIER(S) worst is P--O5': -4.022 &sigma	1 OUTLIER(S) worst is OP1-P-OP2: -4.153 &sigma
A 6	C	0	0.452Å	-	OUTLIER	-	4 OUTLIER(S)

Follow these instructions:  
In your web browser go  
to File >> Save As >>  
Web Page complete



Step 4:  
Repeat and  
Upload

Click this to upload  
your files

Find your files and  
check them

Organize it to the  
VDS Biooproject

The screenshot shows the Google Docs web interface. At the top, the Google logo is on the left, a search bar with 'Home' and a dropdown arrow is in the center, and a blue search button is on the right. Below the search bar is a toolbar with icons for sharing (+), folders, trash, and a 'More' dropdown. On the left side, there is a sidebar with a 'Docs' header, a 'CREATE' button with an upload icon, and a list of navigation options: Home, Starred, Owned by me, All items, Trash, and My collections. Under 'My collections', there is a list of folders including ADAM NGUYEN, CH379H, GroupMeetingSlides, JournalClub, Mentors, Misc, Pics, Protocols, Results&Data, StudentFolders, and VDS Biooproject. The main area on the right displays a list of files and folders. The first item, 'structure-0001.pdb', is highlighted in yellow and has a checkmark in its selection box. Other items include 'VDS Biooproject', 'VDS Pseudoknot', 'RHSGschedule', 'Protein Spectrophotometer Calcs', 'HistoryOfRockStudyGuide', 'Sadhana Balu', and several files related to 'VDSG75frac100111final001Sadhana021612MtPSTP(1329434336)001.res' and '20120216\_SadhanaPSTP\_FPLC.bmp'. At the bottom, there are more files like 'graphvh2-15comp2.png', 'graphvh2-15.png', 'vh2-15-12.xpt', '3IAI\_CA9\_.pdb\_kmvh.gz', and '#7653639\_kmvh.SDF'.

Google

Home x

Docs

CREATE

Home

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Owned by me

All items

Trash

My collections

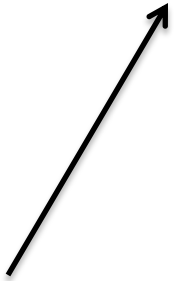
- ADAM NGUYEN
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- VDS Biooproject

Collections shared with me

TITLE

- ☒  structure-0001.pdb
- ☐  VDS Biooproject
- ☐  VDS Pseudoknot Shared VDS Biooproject
- ☐  RHSGschedule Shared
- ☐  Protein Spectrophotometer Calcs Shared Misc
- ☐  HistoryOfRockStudyGuide Shared
- ☐  Sadhana Balu Shared StudentFolders
- ☐  VDSG75frac100111final001Sadhana021612MtPSTP(1329434336)001.res Shared Sadhana Balu
- ☐  20120216\_SadhanaPSTP\_FPLC.bmp Shared Sadhana Balu
- ☐  New Collection Shared Jose Olmos
- ☐  graphvh2-15comp2.png
- ☐  graphvh2-15comp2.png
- ☐  graphvh2-15.png
- ☐  graphvh2-15comp2.png
- ☐  graphvh2-15.png
- ☐  W vh2-15-12.xpt
- ☐  3IAI\_CA9\_.pdb\_kmvh.gz Shared Keyur
- ☐  #7653639\_kmvh.SDF Shared Keyur

# That's it you're done!



Me when you've input your data and  
uploaded your web files

# Your particular structures:

Aldo	2 to 29	Kevan	506 to 533
Amron	30 to 57	Kaarthik	534 to 561
Aakash	58 to 85	Ling	562 to 589
Andrew	86 to 113	Landon	590 to 617
Brandon	114 to 141	Max	618 to 645
Michael	142 to 169	Mihir	646 to 673
Cody	170 to 197	Ramya	674 to 701
Divya	198 to 225	Ruifei	702 to 729
Drew	226 to 253	Suman	730 to 757
Daniel	254 to 281	Stephanie	758 to 785
Fiona	282 to 309	Shreya	786 to 813
Ivy	310 to 337	Shane Ali	814 to 841
Inez	338 to 365	Shashika	842 to 869
James	366 to 393	Sajan	870 to 897
Alex	394 to 421	Urvashi	898 to 925
Jennifer	422 to 449	Zamaria	926 to 953
Janice	449 to 477	Zach	954 to 981
Jonggu	478 to 505		

# Thank you!

